

Ocimene (E)
3779-61-1 | DTXSID8040567

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.31

Global applicability domain: Inside

Local applicability domain index: 5.93e-01

Confidence level: 8.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Myrcene</div> <div>Measured: 4.17</div> <div>Predicted: 4.20</div>	<div>Image not found</div> <div>alpha-Terpinene</div> <div>Measured: 4.25</div> <div>Predicted: 4.25</div>	<div>Image not found</div> <div>sec-Butylbenzene</div> <div>Measured: 4.57</div> <div>Predicted: 4.31</div>
<div>Image not found</div> <div>1-Octene</div> <div>Measured: 4.57</div> <div>Predicted: 4.53</div>		